Modelling and Simulation of Air Pollution: Process Identification, Impact Analysis and Evaluation of Forecast Potential

A Synopsis of the Thesis to be submitted to

MANGALORE UNIVERSITY

for the Award of the Degree of Doctor of Philosophy in

Physics

Submitted by

Jurismita Baruah

Under the Supervision of

Dr. Prashant Goswami

C-MMACS

CSIR Centre for Mathematical Modelling and Computer Simulation
Wind tunnel Road, Bangalore-560037
India

July 2011

1. Title

Modelling and Simulation of Air Pollution: Process Identification, Impact Analysis and Evaluation of Forecast Potential

2. Summary of the Thesis

2.1 Background

Rapid industrialization and increased growth of vehicular traffic especially in the last decades have adversely affected air quality in urban areas, posing threats to environment and health. Extensive research has established that air pollutants affect the health of humans and animals, damage vegetation and materials, reduce visibility and solar radiation and affect weather and climate (Arya 1999; Walsh 1993). Several studies have shown a close relationship between air pollution and mortality (Pope et al. 2002) as well as other ailments (Dockery et al. 1993; Samet et al. 2000). Modelling enables quantitative assessment of the current and future air quality levels, development of control strategies and regulations and evaluation of the effectiveness of control strategy, etc. Reliable simulations of concentrations of pollutants are required for planning and decision support.

This modeling began with studies by Reynolds (1973) for ozone in urbanized areas, with Shir and Shieh (1974) for SO2 in urban areas, and Egan (1976) and Carmichael (1979) for regional scale sulfur. The dispersion of different pollutants using air quality models have been studied for different cities in India in the recent years, e.g. ITO (Gokhale and Khare 2005), Pune, (Dalvi et al. 2005), Coimbatore (Meenakshi and Saseedharan 2004). Kulkarni and Patil (2002) have developed an empirical model to predict the indoor NO2 concentrations in Mumbai. Some commonly used air dispersion models for

vehicular emissions include CALINE 4, IIT Line source Model, HIWAY 2, TEXIN 2 and UAM. The UAM is recommended for urban areas with an ozone problem (Onursal and Gautam 1997).

The daily variations in the atmospheric pollutants depend on both local meteorological processes and various natural as well as anthropogenic sources and sinks. The two major challenges to drive air pollution are a dynamical model that generates the meteorological fields accurately and a species model that realistically represents the sources and the sinks (Main et al. 1994; Moitra and Shukla 1994; Wangkiat et al. 2004) for a location. The modelling of sources and sinks, and representation of effects of natural sources, must be implemented in a location-specific manner, as they vary significantly from region to region. However, there is no dynamical air pollution model for Indian cities like Delhi validated against observations at different time scales. The present thesis describes a dynamical model for daily values of SPM, RSPM, SO2 and NO2 over Delhi.

2.2 Objective and Scope of work

The thesis describes the development of a dynamical model of urban pollution through identification and modelling of various sources, anthropogenic as well as natural, of different air pollutants like suspended particulate matter (SPM), respirable suspended particulate matter (RSPM), nitrogen dioxide (NO2) and sulpher dioxide (SO2) over Delhi. The model has been used to simulate the concentrations of pollutants (SPM, RSPM, SO2 and NO2) over Delhi; the validation has been carried out against daily observations provided by Central Pollution Control Board (CPCB), India. The basic dynamical model of air pollution has been interfaced with forecasts generated by different atmospheric model like General Circulation Model and MM5 model to evaluate potential and skill of the model for forecasting air pollution at different scales. A number

of scenarios that can be effectively controlled with technology or implementable mitigation measures have been examined using the model. Chapter-wise outline of the thesis is provided below.

Chapter 1: Urban Air Pollution

This chapter begins with a brief description of urban air pollution over the Delhi air basin. The chapter describes the basic characteristics of the four pollutants considered in this. This chapter also outlines various sources and effects of these four pollutants.

Chapter 2: Air Pollution Models

This chapter provides the basic procedure to model air pollution and purpose of air quality models. A brief description of commonly used air dispersion models for vehicular emissions as well as some photochemical models is presented here. The major contributions by earlier researchers on different air pollution studies over the Indian region are also briefly described.

Chapter 3: Description of the Dynamical Air Pollution Model

While the basic dynamics of air pollutants (conservation of a scalar quantity) is universal, the evolution of air pollution strongly varies with location and time due to variations in sources and sinks. The variations in the sources and sinks arise from changes in meteorological conditions as well as changes in the response of the human activities to different environmental conditions. Also the sources and sinks, and their relative roles that contribute to the concentration of a species vary with the pollutant. This chapter describes the sources and sinks of the four pollutants, carefully modeled incorporating these factors. In our study, the validation has been carried out against daily values of air pollution over Delhi from observations generated by the Central Pollution Control Board, India (CPCB). The scope and methodology of observations

used for validation of the model are also outlined in this chapter.

Chapter 4: Model Evaluation and Validation: Meteorological Fields from NCEP Reanalysis

The representations of various processes as well as numerical parameters in a model are not unique and need to be carefully calibrated for optimum performance. This chapter describes the hindcasts of daily values of SPM, RSPM, SO2 and NO2 over Delhi by taking the area-averaged fields of daily Reanalysis of NCEP available over a $2.5^0 \times 2.5^0$ global grid as representative meteorological forecasts from a dynamical model. Error statistics, such as average relative percentage error, correlation are used to evaluate the potential of the model for simulating the concentrations of the four pollutants at different time scales.

Chapter 5: Model Evaluation and Validation: Meteorological Fields from GCM Simulation

This chapter provides the simulations and validation of daily values of SPM, RSPM, SO2 and NO2 over Delhi by taking the meteorological fields from variable resolution Global Circulation Model (VR-GCM). The chapter also provides a brief description of VR-GCM, outlining major aspects like the governing equations, numerical integration schemes, various physical parameterizations and grid structure. The initial and boundary conditions required as well the procedure for validation of the numerical simulations are also explained. Finally, an assessment of the impact of GCM generated field with reference to NCEP Reanalysis is presented.

Chapter 6: Comparison of Simulation with MM5 and GCM: Multi-site Evaluation

For simulation and forecasting of air pollution at different points in a city, the atmospheric variables like wind, temperature and precipitation should be taken

from a high resolution meso-scale forecast. Chapter-6 examines the ability of the model to simulate air pollution at different locations and describes the details of the hindcasts of daily values of RSPM, SO2 and NO2 over four locations; ITO, Sirifort, Mumbai and Pune for station-scale forecasts for meteorological parameters such as air temperature, wind and rain using Pennsylvania State University/National Center for Atmospheric Research (PSU/NCAR) meso-scale model version 3 (MM5) and VR-GCM. This chapter also gives a brief description of the MM5 model used for the study. The various aspects of these models such as the initial and boundary conditions required for the numerical simulation are outlined briefly. Objective of this chapter is to evaluate our air pollution model's performance when meteorological data is taken from MM5 model and the model results has been compared with the GCM-derived results.

Chapter 7: Sensitivity Analysis

Simulation of air pollution depends on various components of the model, such as parameterization schemes. Since the dynamics of the concentrations are driven by the meteorological fields, the quality of the simulation also depends on the resolution of the fields of wind, temperature and rain. The impact of increased resolution in the meteorological fields on air pollution simulations is discussed here. Also the impacts of various sources that have been used in our model are described in this chapter.

Chapter 8: Impact Analysis and Quantification

An accurate air pollution simulation model provides an effective tool for impact assessment for various uses. This chapter describes the investigation of pollution loads under different scenarios like doubling of vehicle (and hence also idling time), reducing idling time and reduction in emission rates. Also a measure of the usefulness of the forecasts for application like issues of health advisories is provided by the distribution of error.

Chapter 9: Conclusions and Future Directions.

This chapter includes a summary of the entire study and the major findings. This chapter also discusses some of the limitations and potential improvements of the model. Finally the chapter discusses some of the potential future directions of air pollution modelling.

3. The Dynamical Pollution Model Configuration

The basic dynamics of a species is governed by the continuity equation for a scalar variable (Byun and Schere 2005; Cope and Hess 2005).

$$\frac{\partial s}{\partial t} + u.\frac{\partial s}{\partial x} + v.\frac{\partial s}{\partial y} + w.\frac{\partial s}{\partial z} = S_+ - S_- \qquad (1)$$

where, s represents area-averaged (Delhi) concentration of species in an atmospheric area (μg m^{-3}) and u, v, w are the wind velocity along x, y, z directions respectively. Since the vertical flow w is much smaller than the horizontal flow u and v, and so the transport of pollutants in the vertical due to advection i. e., $w.\frac{\partial s}{\partial z}$ is neglected (Sharan and Gopalakrishnan 2002) at daily scale, although it may have important contribution at short time scales.

The terms S_+ and S_- represent, respectively, sources and sinks of species which we define as:

$$S_+ = S_v + S_W + S_D$$

$$S_- = S_P + S_A$$

where, S_V, S_W and S_D respectively denote contributions to species concentrations due to vehicular exhaust, wind blown dust and domestic appliances.

4. Model Evaluation and Validation with NCEP Reanalysis

4.1 Introduction

Typically, the emissions are released from source, which after entering the atmosphere, depending on the meteorological conditions like wind speed, wind direction, temperature, rainfall, either deposit on a surface or linger in the air in the form of pollution. So air quality models require the data set of meteorological fields to correctly estimate and calculate ambient pollutant concentrations. Hindcasts of daily values of SPM, RSPM, SO_2 and NO_2 over Delhi were carried out by taking the area-averaged meteorological fields of NCEP.

4.2 Results

It can be seen that the model simulations with all sources follow the observed features quite closely, as reflected by a correlation coefficient of above 0.6, highly significant (99% confidence level) for the degrees of freedom involved (Figure 1).

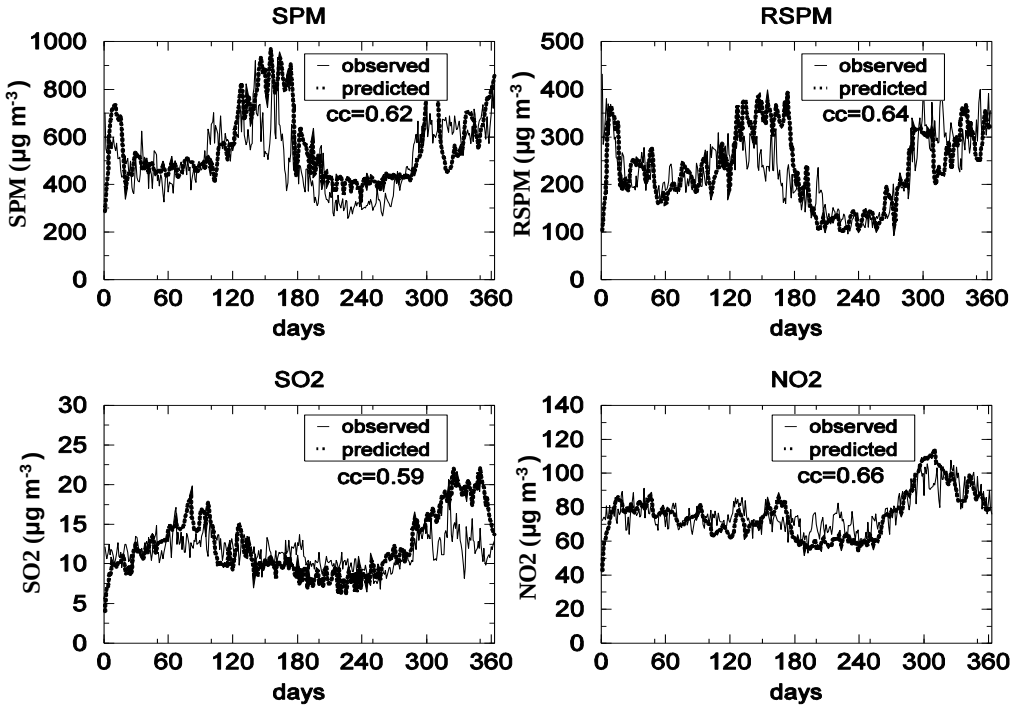

Figure 1: Climatology (2000-2005) of observed (solid line) and simulated (dotted line) values for different pollutants over Delhi as indicated. The simulations are with all sources. The meteorological variables have been adopted from NCEP daily Reanalysis over $2.5^0 \times 2.5^0$ box over Delhi. The observed data is from CPCB.

The daily values of simulated SPM, RSPM, SO_2 and NO_2 also show close agreement with the observations. The correlation coefficients in Table 1 represent, respectively, correlation coefficients between observed and simulated values of daily concentration with only vehicular source and with all sources. These correlation coefficients are significant, except for values less than 0.2, at 99% confidence level for the degrees of freedom involved. Further, correlation

is generally better with inclusion of all sources; however, while positive improvements are, significant in general for SPM, RSPM and SO_2, they are marginal for NO_2. The limited improvement via including non-vehicular sources in simulating NO_2 compared with other species mainly indicates that automobile emission is the biggest contributor to atmospheric NO_2 (Mijling et al., 2009 and Wang et al., 2007).

Table 1: Correlation coefficients between observed and simulated daily SPM, RSPM, SO_2 and NO_2 over Delhi (2000-2005).

Cases	SPM		RSPM		SO_2		NO_2	
	Only vehicle	All sources	Only vehicle	All sources	Only vehicle	All sources	Only vehicle	All sources
2000	0.14	0.35	0.17	0.35	0.32	0.35	0.41	0.49
2001	0.27	0.39	0.41	0.43	0.07	0.21	0.45	0.41
2002	0.13	0.22	0.17	0.21	0.40	0.41	0.30	0.35
2003	0.26	0.51	0.31	0.54	0.15	0.27	0.51	0.49
2004	0.22	0.24	0.25	0.20	0.006	0.30	0.36	0.39
2005	0.20	0.35	0.22	0.50	0.19	0.30	0.19	0.30
Climatology	0.41	0.62	0.54	0.64	0.53	0.59	0.58	0.66

5. Model Evaluation and Validation with GCM fields

5.1 Introduction

The simulation and validation of daily values of SPM, RSPM, SO2 and NO2 were carried out over Delhi by taking the meteorological fields from variable resolution Global Circulation Model (VR-GCM). One of the objectives of the

present work is to also compare and assess the impact of GCM generated field with reference to NCEP Reanalysis used in earlier work. We have therefore used a coarser GCM grid to keep the resolution comparable to the NCEP Reanalysis (250 km).

5.2 Results

5.2.1 Climatology of Observed and Simulated Pollutants

A comparison of climatology (2000-2005) of daily values of SPM, RSPM, SO_2 and NO_2 over Delhi from observation (CPCB) and model simulations for the four species shows (Figure 2) that the model simulations follow the observed features quite closely, as reflected by a correlation coefficient of above 0.6, highly significant (99% confidence level) for the degrees of freedom involved. In particular, the simulated values in each case follow the distinct annual cycle in observed values fairly well. Except NO_2, the observed annual cycles of SPM, RSPM and SO_2 have two maxima: January-February and October-November. The winter maxima (especially during January-February) appears to be significantly controlled by domestic sources. This is consistent with the fact that during May-June, the winds over Delhi turn westerlies, bringing the dust from Thar Desert and arid regions to the west of Delhi (Goyal and Sidhartha 2002). The relatively high values of SPM in the pre-monsoon periods especially after March are attributed to the strengthening of winds associated with the monsoon currents and the resulting dust storms.

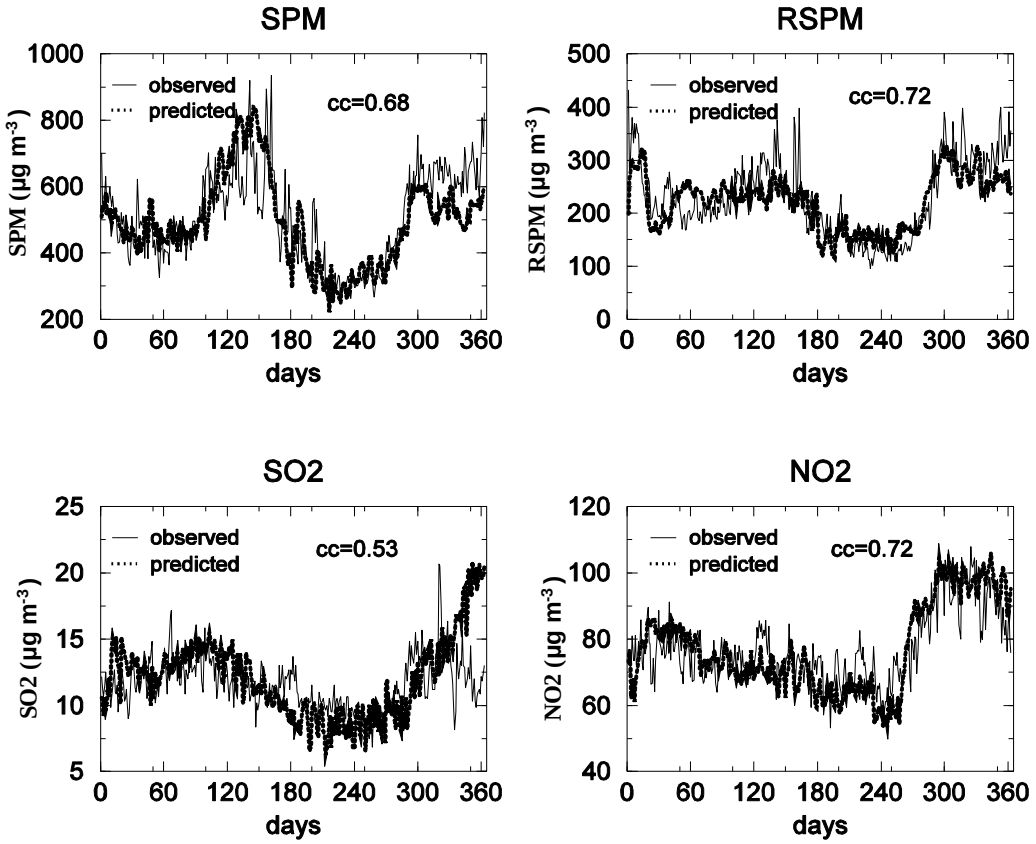

Figure 2: Climatology (2000-2005) of observed (solid line) and simulated (dotted line) values for different pollutants over Delhi as indicated. The meteorological variables have been taken from debiased prediction of gridded model output with the centre of zoom at 77° E and 28° N (Delhi). The observed data is from CPCB.

Consistent with our finding of significant negative correlation between precipitation and SPM, there is a steep fall in SPM in the monsoon months. The sharp fall in SPM in the monsoon season shows the effect of rain on clearing the

atmosphere (Figure 2, top left panel). On the other hand, the observed annual cycle of NO_2 is nearly flat (Figure 2, bottom right panel), indicating no significant correlation with precipitation.

The improvement due to use of GCM-generated fields is most prominent in case of RSPM, with correlation coefficients between observed and simulated RSPM higher with GCM-generated fields than that with NCEP Reanalysis (Table 2) for all the years except 2003. The improvement with GCM-generated fields also significant for SPM except for 2001 and 2003; however, improvement with GCM fields is much more significant than with NCEP Reanalysis. For SO_2 and NO_2, on the other hand, the correlation coefficients for the two cases are comparable (Table 2).

Table 2: Correlation Coefficients between Observed and Simulated daily SPM, RSPM, SO_2 and NO_2 over Delhi (2000-2005).

Cases	SPM		RSPM		SO_2		NO_2	
	NCEP	GCM	NCEP	GCM	NCEP	GCM	NCEP	GCM
2000	0.35	0.40	0.35	0.44	0.35	0.40	0.49	0.54
2001	0.39	0.28	0.43	0.47	0.21	0.18	0.41	0.40
2002	0.22	0.41	0.21	0.38	0.41	0.38	0.35	0.40
2003	0.51	0.45	0.54	0.45	0.27	0.32	0.49	0.48
2004	0.24	0.32	0.20	0.22	0.30	0.33	0.39	0.33
2005	0.35	0.50	0.50	0.54	0.30	0.35	0.30	0.36
Climatology	0.62	0.68	0.64	0.72	0.59	0.53	0.66	0.72

6. Comparison of Simulation with MM5 and GCM: Multi-site Evaluation

6.1 Introduction

Air pollution modeling has seen significant improvements in recent years in general (Cope and Hess 2005; Gery et al.1988; Grivas and Chaloulakou 2006); however, the use of dynamical, in particular, meso-scale models for modeling pollution is relatively still limited in many aspects (Otte et al. 2005; McHerry 2004; Ziomass et al.1995). The meso-scale models today can support horizontal grid spacing down to a few hundreds of meters. We use GCM and mesoscale model MM5 derived fields to evaluate the performances of our model. Here we extend the scope of the model to include four other stations: ITO, Sirifort, Mumbai and Pune. ITO and Sirifort.

6.2 Result

6.2.1 Comparison of Simulation with MM5 and GCM: Location: ITO

Seasonal variations in RSPM, SO2 and NO2 levels over ITO for the year 2010 are depicted in Figure 3. It may be seen that the meteorological fields derived from the two models affect the variability (correlation coefficients in the brackets) in the simulation of pollutant levels over ITO. The model simulation with MM5 model is found to be more accurate than GCM in this case. The correlation coefficients between observed and simulated values are higher with MM5-generated fields than that with GCM-derived fields.

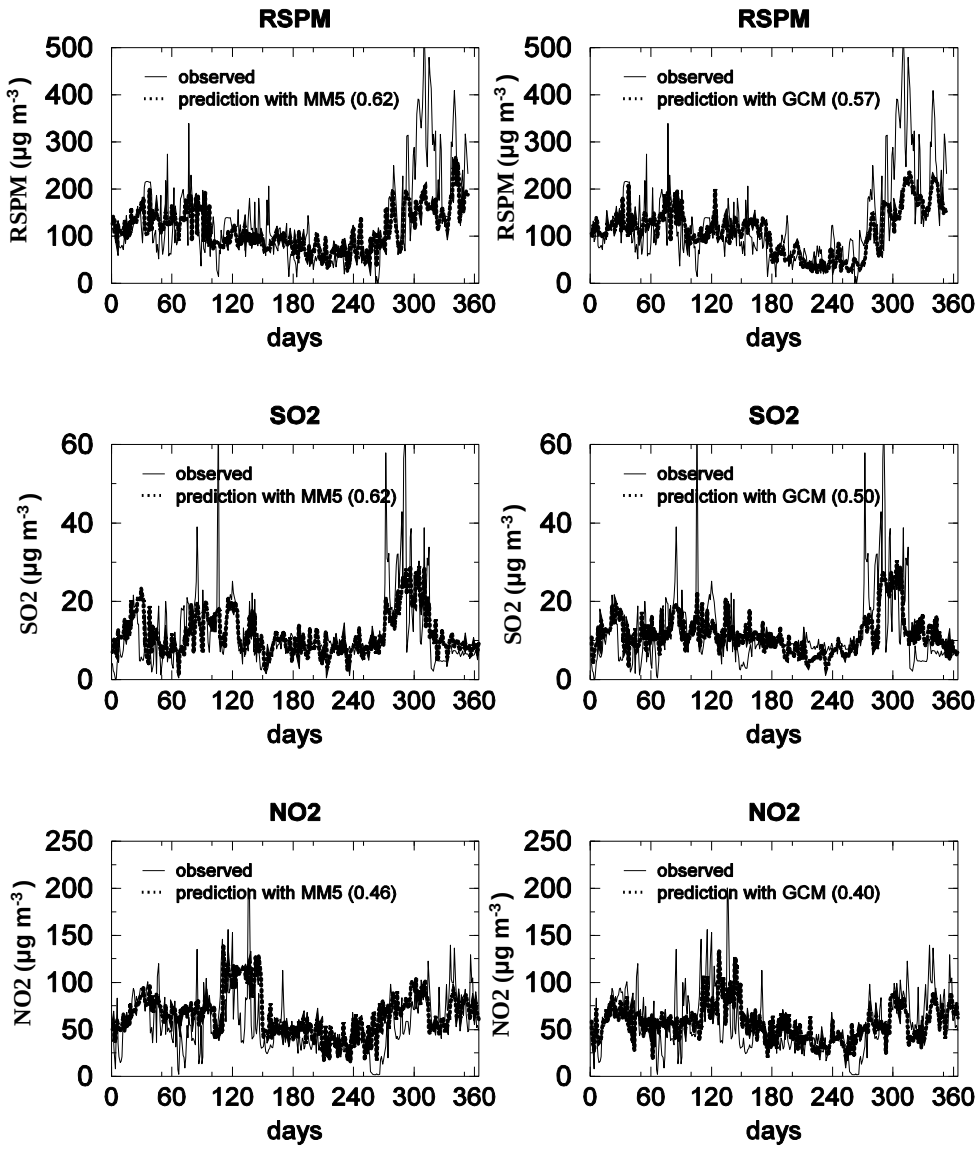

Figure 3: Daily values of RSPM, SO2 and NO2 over ITO for 2010 as indicated. MM5 and GCM derived meteorological fields were used for simulation.

7. Conclusions and Future directions

Air pollution has become a serious problem in urban cities like Delhi. While the present study provides a potential platform for advance forecasting of SPM, RSPM, SO2 and NO2 over a city like Delhi, there are several improvements possible that need to be implemented in a phased manner. Based on our simulations of daily pollutants for six years, it is reasonable to conclude that 24-hour forecasting of pollutants with a dynamical model has significant potential. SPM, RSPM, SO2 and NO2 forecasts generated at high spatio-temporal resolution and interfaced with GIS data can be used to issue advisories as well as to initiate regulatory measures (like traffic planning). Further, such forecasts can be an important input for forecasting events like fog as SPM is an important source of cloud condensation nuclei. One of the most challenging aspects of air pollution modelling is to adequately define the source and the sink functions. Both type and distribution of sources are location specific. It is also necessary to include other minor and seasonal sources of SPM like pollen. Special events like Diwali and Holi can be days on which pollutant source is augmented. Similarly, the vehicular load can show significant day to day modulation depending on a number of factors. Further traffic congestion and thus parameters like idling time and average flow speed of traffic are functions of road width and other parameters. Consideration of these aspects becomes important for location-specific forecasts of pollutants.

8. References:

Arya SP. 1999. Air Pollution Meteorology and Dispersion. Oxford University Press: New York.

Byun, D.W., K. L. Schere, 2005: Review of the governing equations, computational algorithms and other components of the Models-3 Community Multiscale Air Quality (CMAQ) modeling system. *Appl. Mech.Rev*. **59**, 51-77.

Carmichael, G.R., and Peters, L.K., 1979, Numerical simulation of the regional transport of SO2 and sulfate in the eastern United States, Proc. 4 th Symp. on turbulence, diffusion and air pollution, AMS 337.

Cope, M., D. Hess 2005: Air quality forecasting: A review and comparison of the approaches used internationally and in Australia. *Clean Air Environ. Quality*, **39**, 52-60.

Dalvi, M., A Ojha, A. Kesarkar, A. Venkatram, A. Cimorelli and A. Kaginalkar, 2005 : Usage of meteorological model output for pollutant dispersion modelling : A case study for Pune city. National level brainstorming workshop on Indian urban air quality 2005, NEERI, Nagpur, October 24-25.

Dockery, D.W., III C.A. Pope, X. Xiping, J. D.Spengler, J. H. Ware, M. A. Fay, Jr. B.G Ferries and F. E. Speizer, 1993: An association between air pollution and mortality in six US cities. *N. Eng. J. Medicine*, **329**, 1753–1759.

Egan, B.A., K. S. Rao, and A. Bass, 1976: A three dimensional advective-diffusive model for long-range sulfate transport and transformation 7 th ITM, 697, Airlie House.

Gery, M.W., G. Z. Whitten, J. P. Killus, 1988: Development and Testing of the CBM-IV for Urban and Regional Modeling. US Environmental Protection Agency, EPA-600/3-88-012, USA.

Gokhale, S. and M. Khare, 2005: A hybrid model for predicting the carbon monoxide from vehicular exhausts in urban environments, *Atm. Env.*, **39 (22)**, 4025-4040.

Goyal, P., A. Sidhartha, 2002: Effect of winds on SO_2 and SPM concentrations in Delhi. *Atmos. Environ.,* **36**, 2925–2930.

Grivas, G., A. Chaloulakou, 2006: Artificial neural network models for prediction of PM_{10} hourly concentrations, in the Greater Area of Athens, Greece. *Atmos Environ.*, **40**, 1216–1229.

Kulkarni, M.M and R. S. Patil, 2002; An empirical model to predict Indoor NO2 Concentrations. *Atm. Env.*, **36,** 4777-4785.

Meenakshi P. and Saseedharan M. K., 2004: Urban Air Pollution Forecasting with Respect to SPM using Time Series Neural Networks Modelling Approach-A Case Study in Coimbatore City. *J. of Environ Science & Engineering,* **46(2),** 92-101.

Main, S., Sinha S.B., Khan A., Jha C., Verma P.C., Gupta V.S., 1994: Impacts of a coal-fired steam generation plant on ambient SPM levels. *Indian J. Environ. Prot.,* **14 (6),** 406-410.

McHenry, W.F. Ryan, N. L. Seaman, Jr C. J. Coats, J. Pudykiewicz, S. Arunachalam, J. M. Vukovich, 2004: A real time Eulerian photochemical

model forecast system: Overview and initial ozone forecast performance in the northeast U.S. corridor. *Bull Amer. Meteor. Soc*., **85**, 525-548.

Mijling, B., A. R. J. Van Der, K. F. Boersma, M. Van Roozendael, I. De Smedt, H. M. Kelder, 2009: Reductions of NO2 detected from space during the 2008 Beijing Olympic Games. *Geophys. Res. Lett.*, **36**, L13801.

Moitra, J., N. Shukla, 1994: Determination of stack gas velocity and total suspended particulate matter from source emissions. *Indian J. Environ. Prot.* **14 (10),** 729-736.

Onursal, Bekir and Gautam, Surhid 1997: Vehicular air pollution: Experiences from seven Latin American urban centers. Publisher- World Bank, **373,** 282p.

Otte, T., and Coauthors, 2005: Linking the Eta model with the Community Multiscale Air Quality (CMAQ) modeling system to build a national air quality forecasting system. *Wea Forecasting*, **20**, 367-384.

Pope, C.A., Burnett, R.T., Thun, M.J., Calle, E.E., Krewski, D., Ito, K., Thurston, G.D., 2002: Lung cancer, cardio-pulmonary mortality, and long-term exposure to fine particulate air pollution. *J of the American Medical Assoc.*, **287 (9)**, 1132–1141.

Reynolds, S., P. Roth, and J. Seinfeld, 1973: Mathematical modeling of photochemical air pollution. *Atm. Env*, 7.

Samet, J.M., S.L. Zeger, F. Dominici, F. Curriero, I. Coursac, D.W. Dockery, J. Schwartz, A. Zanobetti, 2000: The national morbidity, mortality, and air pollution study. Part II.: Morbidity, mortality and air pollution in the United States. Health Effects Institute Research Report 94; Part II.

Shir, C.C. and L.J. Shieh, 1974, A generalized urban air pollution model and its application to the study of SO2-distribution in the St. Louis Metropolitan area, *J. Appl. Met.*, **19**, 185-204.

Sharan, M., S. G. Gopalakrishnan, 2003: Mathematical modelling of diffusion and transport of pollutants in the atmospheric boundary layer. *Pure and Applied Geophysics*, **160**, 357-394.

Walsh, M.P., 1993. Highway vehicle activity trends and their implications for global arming. The United States in an international context. In: Greene, D.L., Santini, D.J. (Eds.), Transportation and Global Climate Change. American Council for an Energy Efficient Economy, Washington.

Wang, Y.X., M. B. McElroy, K. F. Boersma, H. J. Eskes, J. P. Veefkind, 2007: Traffic Restrictions Associated with the Sino-African Summit: Reductions of NOx Detected from Space, *Geophys. Res. Lett.*, **34**, L08814.

Wangkiat, A., N. W. Harvey, H. Garivait, S. Okamoto, 2004: Source contribution of atmospheric aerosols in Bangkok metropolitan area by CMB_8 receptor model. *Int. J. Environ. Pollut.* (IJEP), **21(1),** 80-96.

Ziomass, I.C., M. Dimitrios, S. Z. Christos, F. B. Alkiviadis, 1995: Forecasting peak pollutant levels from meteorological variables. *Atmos. Environ.*, **29**, 3703–3711.

9. List of Publications

i. Goswami, P., and J. Baruah, 2008: Simulation of Daily Variation of Suspended Particulate Matter over Delhi: Relative Roles of Vehicular Emission, Dust and Domestic Appliances. *Mon. Wea. Rev.,* **136(9),** 3597-3607.

ii. Goswami, P., and J. Baruah, 2010: Urban air pollution: process identification, impact analysis and evaluation of forecast potential. *Meteorol. Atmos. Phys.,* **110**, 103-122.

Signature of the Candidate **Signature of the Guide**

(Jurismita Baruah) (Dr. P. Goswami)